

MONTE CARLO DETERMINATION OF THE UNCERTAINTY OF EFFECTIVE AREA AND DEFORMATION COEFFICIENT FOR A PISTON CYLINDER UNIT

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Abstract:

This paper describes the approach made to describe the uncertainty on the area at zero pressure (A_0) and on the deformation coefficient (λ) of piston-cylinders used for pressure definition. We perform the Monte-Carlo simulation for an ordinary least squares (OLS) as well as for a weighted least squares (WLS) and a generalized least squares (GLS). We also introduce an innovative technique to improve the results obtained by WLS in order to get close to the quality obtained using GLS. We discuss the different situations that guides to the best choice between OLS, WLS and GLS.

Keywords: Monte-Carlo, uncertainty, pressure balance, piston-cylinder

1. INTRODUCTION

Traditionally, pressure laboratories have an uncertainty on the effective area determined by cross floatation based on the uncertainties on the influence factors and the sensitivity coefficients. [1-3]. The uncertainty on the area at zero pressure (A_0) and the deformation coefficient (λ) determined by least squares is not trivial to obtain by the technique of the sensitivity coefficients. The project Euramet 1125 [4] described the results obtained by several national metrology institutes in Europe for a set of data, simulating measurements affected by known uncertainties. Alternative techniques have been recently proposed to improve the uncertainty [5-7]. We explore the uncertainty of the determination of effective area at zero pressure and deformation coefficient based on Monte-Carlo simulation of the calibration process and the determination of λ and A_0

2. GOAL OF THIS WORK

METAS and LPEE-LNM performed recently a bilateral comparison of piston-cylinder units. We wanted not only to compare the effective area, at a given pressure, but also the values for A_0 and λ

obtained by least squares calculation on the set of measurements. A Monte-Carlo simulation is an efficient and mathematically correct way to assess the uncertainty of a value obtained using a least squares calculation. We are confronted to inhomogeneous uncertainties on the effective area depending of the pressure at which the effective area is measured, leading to heteroscedasticity on the residuals. We also have a correlation in the error of the mass used on each pressure balance as the mass used for the realisation of the first pressure step remains on the pressure balance for the second pressure step and so on for each successive pressure step. The whole set of mass is also calibrated against the same reference and the different pieces of charge are correlated to some degree.



Figure 1: Setup used for the determination of the piston-cylinder effective area. The reference pressure balance, on the left, is working with gas and the pressure balance under calibration, on the right, is working with oil.

3. DETERMINATION OF A_0 AND LAMBDA

In pressure metrology we determine the effective area of a piston cylinder unit (PCU) at different pressure points by cross floatation [2-3]. Based on these measurements we want to determine the effective area at zero pressure (A_0) and the deformation coefficient (λ), in order to have a model of the deformation of the PCU under pressure. The area of the PCU at a given pressure is the given by:

$$A(p) = A_0(1 + \lambda p) \quad (1)$$

Because we have only two free parameters to determine but have measurements performed at a larger number of pressure points it is convenient to use a least square approach to solve this equation. It is convenient to rewrite (1) the following way:

$$A(p) = A_0 + b \cdot p \quad (2)$$

Where b is in fact $A_0^* \lambda$.

3.1. Least squares determination

The model used for the relation between the set of measurement, the deformation coefficient and the effective area at zero pressure is as follow:

$$\begin{pmatrix} 1 & p_1 \\ \vdots & \vdots \\ 1 & p_n \end{pmatrix} \cdot \begin{pmatrix} A_0 \\ b \end{pmatrix} = \begin{pmatrix} A(p_1) \\ \vdots \\ A(p_n) \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}. \quad (3)$$

Where the p_i are the pressure steps at which we determined the effective area $A(p_i)$. The value A_0 is the effective area at zero pressure and b is the increase of area per unit pressure due to deformation and these two values are the unknown of the system. The ε_i are the residual that we will minimise using the least square equation.

We can rewrite the equation 2 using the following matrix definition:

$$XC = Y + E \quad (4)$$

We introduce a weighting matrix that multiplies the terms of the equation on the left and on the right.

$$V^{-1}XC = V^{-1}Y \quad (5)$$

The matrix V is the weighing coefficient. V is an identity matrix in the case of ordinary least square (OLS). V is a diagonal matrix with coefficients proportional to the uncertainty of $A(p_i)$ or to the square of the uncertainty of $A(p_i)$ in the case of the weighted least squares according to respectively the uncertainty (WLS-U) or the uncertainty squared (WLS-U2). V is the matrix of variance and covariance of the $A(p_i)$ in the case of generalised least squares (GLS). For simplicity of writing we define the matrix W as V^{-1} .

We then solve the equation by multiplying by X' , the transpose of X on the left side:

$$X'V^{-1}XC = X'V^{-1}Y \quad (6)$$

And finally we multiply by $(X'V^{-1}X)^{-1}$ on the left side and obtain the solution of the equation system:

$$C = (X'V^{-1}X)^{-1} * X'V^{-1}Y \quad (7)$$

4. MONTE CARLO SIMULATION

The Monte-Carlo simulation reproduces the errors obtained when performing the determination of the effective area of a piston-cylinder using the cross-floating technique. The effective area for a given pressure step is obtained by using the usual

equation of effective area determination. In a first step we calculate the pressure generated by the reference pressure balance by the j th pressure step:

$$p_j = \frac{\sum_i m_i g (1 - \rho_a / \rho_{mi})}{A_{R0} (1 - \lambda p) (1 + (\alpha_p + \alpha_c)(t - t_r))}. \quad (8)$$

And then we calculate the effective area of the piston under test.

$$A_{pj} = \frac{\sum_i m_{ij} g (1 - \rho_{aj} / \rho_{mij})}{p_j (1 + (\alpha_p + \alpha_c)(t - t_r))}. \quad (9)$$

In our model there is 9 pressure steps and we assume that the measurement is repeated 10 times in order to determine the effective area. A set of measurement comprises the 90 measurement resulting from the 9 pressure steps repeated ten times.

We repeat the calculation to obtain 10'000 measurement sets in order to perform the uncertainty calculation on A_0 and λ of the piston under calibration.

The errors we generate in the Monte-Carlo simulation are supposed to depict as close as possible the reality of the metrological process. All influence factors have an error contribution considered constant in the whole set of measurements that do not change from one pressure step to the next one. Some influence factors are considered to have an error contribution that does change at each pressure step. This is the case for influence factors that need a new measurement at each pressure step.

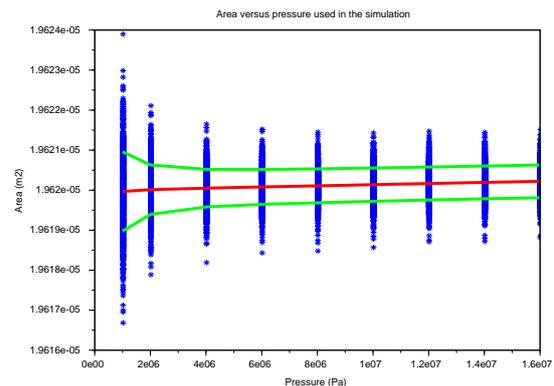


Figure 2: Plot (blue stars) of the effective area obtained in the Monte-Carlo simulation. The red line is the average value of the effective area and the green curves are placed at plus and minus the standard deviation.

4.1. Generation of the set of data

As illustration of the numerical technique we simulate a piston of 2 bar/kg working with air used to calibrate a piston of 5 bar/kg working with oil.

We perform the calibration at 1 MPa, 2 MPa and then each 2 MPa up to 16 MPa. The values and respective uncertainties type A and B are given in table 1. We assume for all the uncertainties a normal distribution in our simulation.

The simulation is performed using scilab 6.1.0 [9] on a small computer running a 64 bits operating

system like Linux or Windows. The generation of the 10'000 sets of data, the resolution of the least squares equations for the different weighting schemes and some statistical calculations takes about 2 minutes.

Table 1: Values and related uncertainties of type A and type B used in the simulation.

Influence factor	Abreviation	Value	Uncertainty type B	Uncertainty type A
Effective area reference piston	$A_{0,ref}$	$4.905 \times 10^{-5} \text{ m}^2$	$9.64 \times 10^{-10} \text{ m}^2$	
Deformation coefficient reference	λ_{ref}	$7.0 \times 10^{-13} \text{ Pa}^{-1}$	$1.0 \times 10^{-13} \text{ Pa}^{-1}$	
Effective area piston to calibrate	$A_{0,cal}$	$1.962 \times 10^{-5} \text{ m}^2$		
Def. coefficient piston to calibrate	λ_{cal}	$7.0 \times 10^{-13} \text{ Pa}^{-1}$		
Thermal expansion coeff. reference	α_{ref}	9 ppm/°C	1 ppm/°C	
Therm. Exp. coeff. Piston to calibrate	α_{cal}	9 ppm/°C	1 ppm/°C	
Mass used on the reference piston	$M_{i,ref}$	5 kg	50 mg	
		10 kg	50 mg	
Mass used on the piston to calibrate	$M_{i,cal}$	2.0 kg	20 mg	
		4.0 kg	20 mg	
Height of the oil column	Δh	0 m	0.05 m	0.003 m
Temperature of the reference piston	T_{ref}	22 °C	0.1 °C	0.1 °C
Temperature of the piston to calibrate	T_{cal}	22 °C	0.1 °C	0.1 °C
Density of the mass used on the ref.	ρ_{Miref}	7950 kg/m ³	71 kg/m ³	
Dens. of the mass used on the sample	ρ_{Mical}	7950 kg/m ³	71 kg/m ³	
Density of air	ρ_{air}	1.2 kg/m ³	0 kg/m ³	0.005 kg/m ³

5. DETERMINATION OF THE WEIGHTING MATRIX

The weighting matrix V used in the least square calculation according to equation 5 can be defined of different manners [8]. The simplest way is to take a diagonal matrix with 1. This is the situation of ordinary least squares determination (OLS).

$$v_{ij} = 0: i \neq j, \quad v_{ii} = 1 \quad (10)$$

Traditionally people working on the determination of the parameters of PCU use a diagonal weighting matrix in which the values of the elements on the diagonal are related to the uncertainty of the effective area obtained at a given pressure step. (WLS-U)

$$v_{ij} = 0: i \neq j, \quad v_{ii} = u(A(p_i)) \quad (11)$$

Another solution consists in a weighting matrix in which the diagonal elements are determined by the square of the uncertainty of the effective area at a given pressure. (WLS-U2)

$$v_{ij} = 0: i \neq j, \quad v_{ii} = u^2(A(p_i)) \quad (12)$$

Finally we can determine the matrix V using the variance and covariance of the effective area at the different pressure steps. This approach is

susceptible to provide the best uncertainties but is difficult to implement because the determination of the covariance can be challenging. In our situation we have a large set of simulated data through the Monte-Carlo calculation and are able to calculate the covariance based on the set of data at our disposal. (GLS)

$$v_{ij} = cov(A(p_i), A(p_j)): i \neq j, \quad (13)$$

$$v_{ii} = u^2(A(p_i))$$

Until now all the matrices we have considered are based on the uncertainties observed on the effective area of the PCU. In a recent publication [6], P. Otal introduced the notion of matrix coefficients based on the uncertainty of $\tilde{A}(p)$ which is calculated assuming only the uncertainty contributions on the effective area that are pressure dependant and contribute to heteroscedasticity. In our model we take into account the contribution of the height of the oil column (Δh) and the deformation coefficient of the reference PCU (λ_{ref}). The plot of the $\tilde{A}(p)$ and their standard deviation is shown on Fig. 3.

We are able, based on the uncertainty of $\tilde{A}(p)$, to define the following matrices used in the least squares determination.

A weighted least squares based on the uncertainty of $\tilde{A}(p)$ as explained in [6] (WLS-U \tilde{A}):

$$v_{ij} = 0: i \neq j, \quad v_{ii} = u(\tilde{A}(p_i)) \quad (14)$$

A weighted least squares based on the square of the uncertainty of $\tilde{A}(p)$ (WLS-U2 \tilde{A}):

$$v_{ij} = 0: i \neq j, \quad v_{ii} = u^2(\tilde{A}(p_i)) \quad (15)$$

Finally, we can also define a generalised least squares matrix based on $\tilde{A}(p)$ (GLS- \tilde{A}):

$$v_{ij} = cov(\tilde{A}(p_i), \tilde{A}(p_j)): i \neq j, \quad (16)$$

$$v_{ii} = u^2(\tilde{A}(p_i))$$

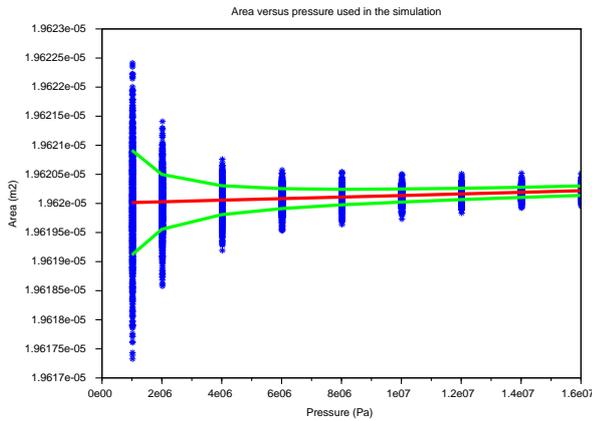


Figure 3: Plot (blue stars) of the effective area obtained in the Monte-Carlo simulation taking into account the uncertainties related to the oil column and the deformation coefficient. The red line is the average value of the effective area and the green curves are placed at plus and minus the standard deviation.

It is interesting to note that the diagonal elements of the matrix are similar in the equation 12 and 13 as well as in equation 15 and 16.

The coefficients of the diagonal of the matrix W are summarised in Table 2 and show the relative importance given to the different measurements.

Table 2: Elements w_{ii} used according to the different weighing schemes. A normalisation has been applied so that the larger element is equal to one.

	WLS -U	WLS -U2	WLS -U \tilde{A}	WLS -U2 \tilde{A}
w_{11}	0.395	0.157	0.086	0.008
w_{22}	0.644	0.414	0.170	0.029
w_{33}	0.861	0.743	0.325	0.106
w_{44}	0.937	0.877	0.468	0.219
w_{55}	0.968	0.938	0.600	0.361
w_{66}	0.984	0.968	0.722	0.521
w_{77}	0.992	0.984	0.830	0.689
w_{88}	0.997	0.993	0.923	0.851
w_{99}	1.000	1.000	1.000	1.000

5.1. Uncertainties on A_0 and λ

We applied the different weighing schemes to our set of data. We managed to obtain an average value for A_0 and λ similar to the nominal value for all the weighting matrices demonstrating that the technique is correct. The standard deviation obtained on A_0 and λ greatly depends on the weighting scheme selected. The results summarised on table 3 show that the GLS techniques delivers the best uncertainties. Weighting least squares based on the square of the uncertainty are more performant than those based on the uncertainty. The most interesting result is that the uncertainty on A_0 and λ for the WLS based on $u^2(\tilde{A}_p)$ is the closest from the results obtained with a GLS approach. It is also interesting to note that the GLS approach based on $\tilde{A}(p)$ delivers results similar with the GLS based on $A(p)$.

Table 3: Values and respective uncertainties obtained for the area at zero pressure and the deformation coefficient for the PCU under calibration, for different least squares techniques.

	A_0	λ
Nominal value	$1.962 \times 10^{-5} \text{ m}^2$	$0.70 \times 10^{-12} \text{ Pa}^{-1}$
u(OLS)	36 ppm	$2.20 \times 10^{-12} \text{ Pa}^{-1}$
u(WLS-U)	31 ppm	$1.70 \times 10^{-12} \text{ Pa}^{-1}$
u(WLS-U2)	28 ppm	$1.35 \times 10^{-12} \text{ Pa}^{-1}$
u(GLS)	20 ppm	$0.36 \times 10^{-12} \text{ Pa}^{-1}$
u(WLS-U \tilde{A})	28 ppm	$1.21 \times 10^{-12} \text{ Pa}^{-1}$
u(WLS-U2 \tilde{A})	24 ppm	$0.74 \times 10^{-12} \text{ Pa}^{-1}$
u(GLS- \tilde{A})	20 ppm	$0.35 \times 10^{-12} \text{ Pa}^{-1}$

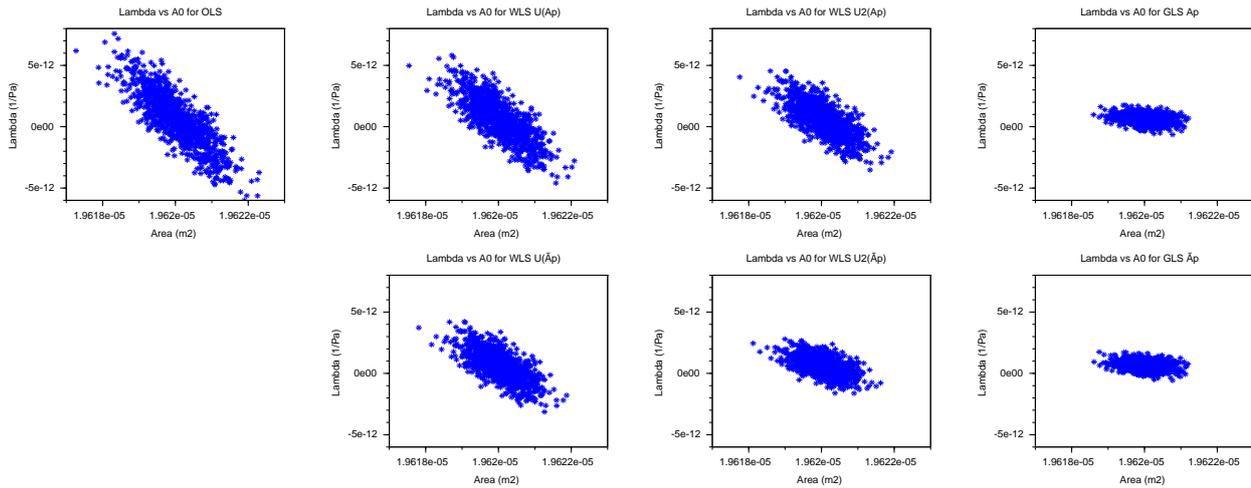
The plot of λ versus A_0 for the different least square weighting matrices, depicted in Fig. 4, shows the uncertainties and correlation obtained with the different least squares approximations.

In order to assess the independence of the uncertainties on A_0 and λ , we calculated the correlation between the two parameters for the different weighing matrices used in the least square calculation. The results, presented on table 4, show that the correlation is relatively high when OLS is used but can be decreased to almost negligible amount in the case of a GLS approach. The correlation for the WLS according to $u^2(\tilde{A}_p)$ is the best value if we exclude the GLS.

Table 4: Correlation between A_0 and λ for the different weighing matrices tested in the simulation.

Weighting matrix	Correlation $A_0 - \lambda$
OLS	-0.83
WLS-U	-0.77
WLS-U2	-0.71
GLS	-0.28
WLS-U \tilde{A}	-0.69
WLS-U2 \tilde{A}	-0.55
GLS- \tilde{A}	-0.27

Figure 4: Plot of λ versus A_0 for different least square calculation: From left to right, top: OLS, WLS-U, WLS-U2 and GLS, bottom: WLS_U \tilde{A} , WLS_U2 \tilde{A} , GLS_ \tilde{A} .



6. SUMMARY

We applied successfully a Monte-Carlo simulation to determine the uncertainty on A_0 and λ determined by cross floating of pressure balances. Our numerical simulation has been used to optimise the weighting matrix used in the determination of A_0 and λ . The raw data from the Monte-Carlo simulation have been used to determine the covariance between the effective areas determined at two different pressure.

We have shown that an improvement of the weighting matrix proposed by Otal and Al. is able to provide an uncertainty close to what is obtained using a generalised least squares approach.

The authors want to thank the PTB for providing this collaboration opportunity between METAS and LPEE-LNM through the project "Promotion of quality-assurance capabilities and services in the Maghreb to strengthen international trade". We want to thank Dr. Kilian Marti for his help in correcting the manuscript.

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